Entanglement-Entropy for Groundstates, Low-lying and Highly Excited Eigenstates of General (Lattice) Hamiltonians

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Abstract

We investigate the question of entanglement-entropy on a broad scale, that is, a large class of systems, Hamiltonians and states describing the interaction of many degrees of freedom. For calculational convenience we study primarily systems defined on large but finite regions of regular lattices. We show that general vector states, being not related to some short-range Hamiltonian do not lead in the generic case to an area-like behavior of entanglement-entropy. The situation changes if eigenstates of a Hamiltonian with short-range interactions are studied. We find three broad classes of eigenstates. Global groundstates typically lead to entanglement-entropies of subvolumes proportional to the area of the dividing surface. Macroscopically excited (vector)states have in the generic case an entanglement-entropy which is proportional to the enclosed subvolume and, furthermore, display a certain Gibbsian behavior. Low-lying excited states, on the other hand, lead to an entanglement-entropy which goes usually with the logarithm of the enclosed subvolume. Our analysis is mainly based on a combination of concepts taken from the perturbation theory of Hamiltonians and certain insights coming from the foundations of quantum statistical mechanics.

1 Introduction

The microscopic origin of entropy in, for example, black hole phyics and the so-called *area law* is still to some extent kind of a mystery. Or more precisely, there exist a variety of different explanations. For a nice discussion in form of a Galilean trialogue see [1], a collection of theses can also be found in [2]. Of perhaps even more interest is the proposed *holographic principle* (and the range of its validity), which pulls back the emergence of entropy on a very fundamental level of physics, that is, "empty" space (-time) and its *vacuum fluctuations*. We do not attempt to give a complete list of references (as we focus in the following on a related but slightly different question), cf. for example the nice review [3] and the many references therein.

What is at least clear is that the black hole horizon divides space-time into *exterior* and *interior* regions. Hence, one might venture the idea that a basic role in this question should be played by some form of *entanglement* of two (in some macroscopic respect) separated regions. Such a form of entanglement can however be realized on one or the other level of our theoretical description, ranging from more ordinary ones (standard quantum mechanics or quantum field theory) to more pristine ones (e.g. the notorious Planck scale). On this point people widely disagree at the moment. As to our personal point of view, we think that the holographic principle indicates a drastic change of the statistical mechanical preassumptions usually taken for granted on the more ordinary scales as e.g. *locality*, good clustering conditions or sufficient decay of correlations etc., if one enters the fundamental regime of the Planck scale. Some very sketchy remarks can be found at the end of [4], a more detailed analysis is forthcoming. Be that as it may, one should emphasize the following:

Observation 1.1 *The following two situations are different from a logical point of view, for one, entanglement-entropy induced by a fixed global state as e.g. the groundstate of a given Hamiltonian, for another, the maximally possible quantum of entropy or information which can be stored in a given volume, the question which is adressed in the holographic principle. In the latter case also the highly excited states of a Hamiltonian should be investigated, a problem we explicitly adress in the following sections.*

In any case, in a first step, it seems to be useful to investigate ordinary models of quantum (field) theory and see to what extent their entropic behavior reflects some of the properties condensed in notions like area law and/or holographic principle. To make the problem more accessible, one can start with the investigation of systems of many degrees of freedom living on a

large regular lattice (of arbitrarily small but finite lattice constant). In [5] or [6], large arrays of coupled harmonic oscillators and their respective groundstates have been studied, with some sort of continuum limit performed in the end, yielding the vacuum state of e.g. a Klein-Gordon field theory. Note however that taking a continuum limit is quite delicate since, in order to get a finite result, some form of *cut-off* is necessary (as to possible interesting applications to quantum field theory see for example [7]).

As everybody knows, the harmonic oscillator is an extremely well-behaved quantum system. The same holds for regular arrays of coupled harmonic oscillators. There exists a large arsenal of methods to extract useful information from these model systems. But nevertheless, the question of *entanglement-entropy* of, say, the groundstate of this well-behaved model system turns already out to be quite intricate (see the above cited two papers). This may, among other things, have its roots in the observation that the concept of entanglement-entropy and its quantitative behavior is not so easy to visualize, one reason being, that it is not a truely local concept.

It was found that if one divides a large volume, V, into $V_1 \cup V_2$ and restricts the groundstate, Ψ_0, over V to the subvolumes V_1, V_2, the corresponding *density matrices*, W_1, W_2, have an entropy, $S = -\sum w_i \ln w_i$, which is proportional to the area of the dividing surface between V_1 and V_2! One may therefore speculate that this observation has something to do with the area law in black hole physics and corresponding arguments were provided in the two above cited papers.

If one persues such an idea, various questions immediately suggest themselves.

i) What properties make the groundstate of the Hamiltonian of a large system (i.e., many degrees of freedom being involved) a particular state; if there exist any criteria in this context. Put differently, what particular property of a global vectorstate (pure state) influences the entropic behavior of the *partial traces*, W_1, W_2?

ii) In what respect does the picture change if we go over to *lowly* or *highly excited* eigenstates of such a Hamiltonian?

iii) Is the result, found for an array of harmonic oscillators, generic, that is, is it to a high degree independent of the particular model system being used and what are the really important prerequisites?

These are the questions we will adress in the following sections.

We begin by defining the general framework of systems, living on large regular lattices. The adequate mathematical structure is the tensor product structure of corresponding Hilbert spaces, states, and operators. That is, at each lattice site, x_i, sits a finite or infinite dimensional Hilbert space, $\mathcal{H}_i$,

with in general all $\mathcal{H}_i$ being isomorphic. Systems, restricted to large but finite (macroscopic) volumes, V, are then built by forming tensor products of these local $\mathcal{H}_i$ with $x_i \in V$. The same applies to states and, for example, Hamiltonians on V.

We then discuss several general properties of the notion of *entanglement-entropy*, that is, what happens if for example a vectorstate over V is traced over a subvolume V_2 to yield a new state (in fact a *density matrix*), W_1, on V_1 with $V = V_1 \cup V_2$. We show among other things that a Gibbs state over V_1 can always be extended to a pure vector state, Ψ, on V by enlarging the system on V_1 with $V = V_1 \cup V_2$. That is, the Gibbs state is now the partial trace of a global vectorstate. As, typically, such Gibbs states have an entropy which is proportional to the volume, V_1, this shows that, in general, entanglement-entropy does *not* go with the area of the surface, dividing V_1 and V_2. We learn from this that, in order to get such a special result, some extra specifications are called for.

This observation teaches us yet another lesson. One sometimes hears the argument that entanglement-entropy has to go with the area of the dividing surface as this is the only quantity which is the same for both volumes, V_1 and V_2 while the volumes can of course differ from each other (note that, perhaps a little bit surprisingly, entanglement-entropy is always the same forV_1 and V_2). This argument is obviously incorrect. What will in general happen is that we have something like the following

$$S(W_1) = \alpha_1 \cdot |V_1| = \alpha_2 \cdot |V_2| = S(W_2) \tag{1}$$

with W_1, W_2 the density matrices representing the total state, Ψ, on V_1, V_2 respectively. That is, both entropies may go with the volume but with certain adjusting prefactors.

At the end of this section we introduce a certain *coarse-grained* version or approximation of the notion of entanglement-entropy for the subvolumes V_1, V_2, which, in some sense, resembles kind of a microscopic ensemble version of entropy. In our particular case it is related to the logarithm of the dimension of certain Hilbert subspaces onto which the pure vectorstate is primarily projected. This is an important simplification: While the original standard notion of entropy, $S := -\sum w_i \cdot \ln w_i$, is deceptively simple at first glance, this is a very missleading impression. Even in the few cases where the Boltzmann weights, w_i, are known, what is usually more important is their (frequently huge) degeneracy and/or the local density of states. Therefore we surmise that the situation in the harmonic oscillator case is quite atypical.

As we treat the problem of entanglement-entropy on a very broad scale (as far as the class of admissible models is concerned), it is out of the question to work with the original concept of entropy. We need expressions which, while giving perhaps less detailed information, lead to the same results as far as estimates of the kind "order of..." on a logarithmic scale are concerned.

For the same reason (a large class of different admissible Hamiltonians) we develop in section 4 in quite some detail various concepts belonging to the perturbational analysis of Hamiltonians. This turns out to be a very intricate subject matter in our context. The main reason is that, due to the dense distribution of eigenvalues typical for Hamiltonians of a large number of degrees of freedom, ordinary perturbation theory is of only a very limited value.

In the last three sections we then deal with our main topic in a more quantitative way. In section 5 we treat the case of the groundstate of a Hamiltonian with *finite range* interactions. In the following section we analyse the situation for eigenstates which are highly excited, that is, for energies which are a macroscopic distance apart from the groundstate energy. In the last section we study, on the other hand, eigenvalues of the Hamiltonian which lie in the vicinity of the groundstate energy. We find the following:
i) Groundstates come with an entanglement-entropy which is proportional to the area of the dividing surface.
ii) Highly excited states lead in the *generic* case to entanglement-entropies which go with the volume of the system. Furthermore, the restriction of the pure vectorstate to the respective subvolumes share a couple of properties with ordinary temperature states. As for more detailed qualifications see the corresponding section.
iii) Low-lying excited eigenstates states have an entanglement-entropy which goes roughly with the logarithm of the corresponding volume.

To sum up what we think have been important ingredients in our analysis, the arguments strongly rely on the finite range of the interactions, that is some version of *locality*. As to the applied methods, two tools stand out. First, a combination of various perturbational arguments, second, a couple of technical ideas which have proved their worth already in the foundations of *statistical mechanics*.

We add the remark that there exist several papers in which entanglement-entropy is studied for a certain class of (typically low-dimensional) solvable models by using quite particular methods. The general aim of these papers is however for the most part a different one, we mention [8],[9],[10]. We note also that in the following we do not treat systems which are in a *quantum-critical state*, i.e. have correlations extending to infinity.

2 A Brief Description of the Formal Framework

To avoid irrelevant complications it is reasonable to choose as the general context discrete dynamical models living on a regular lattice, $\mathbb{Z}_a^d$, with lattice constant a and space dimension d. The points of the lattice are denoted by x_i, the Hilbert space sitting at x_i by $\mathcal{H}_i$. $\mathcal{H}_i$ may be finite or infinite dimensional (as is for example the case for an array of harmonic oscillators). If all the $\mathcal{H}_i$ have the same finite dimension it is denoted by D.

We are usually interested in large but finite subsets of $\mathbb{Z}_a^d$, denoted by V, comprising a finite number of lattice points, $x_i \in V$. For illustrative purposes V may be chosen as a d-dimensional cube of side length L, containing $N_V = (L/a)^d$ lattice points. The general case of regions of arbitrary shape can of course be treated in more or less the same way apart from some (irrelevant) numerical details. The Hilbert space, $\mathcal{H}_V$, living over V has a tensor product structure

$$\mathcal{H}_V = \bigotimes_{x_i \in V} \mathcal{H}_i \tag{2}$$

spanned by tensor-monomials

$$v = v_1 \otimes \cdots \otimes v_{N_V} \ , \ v_i \in \mathcal{H}_i \tag{3}$$

If one chooses a basis, $e_i^{l_i}$, in each $\mathcal{H}_i$, general vectors in $\mathcal{H}_V$ are linear combinations of the basic vectors

$$e_1^{l_1} \otimes \cdots \otimes e_{N_V}^{l_{N_V}} \ , \ 1 \leq l_i \leq D \tag{4}$$

(if the dimension of $\mathcal{H}_i$ is finite). In that case the dimension of $\mathcal{H}_V$ is D^{N_V}. The scalar product on $\mathcal{H}_V$ is given by

$$(v_1 \otimes \cdots \otimes v_{N_V} | v'_1 \otimes \cdots \otimes v'_{N_V}) := \prod_{x_i} (v_i | v'_i) \tag{5}$$

and (multi)linearly extended.

Now we come to the definition of interaction, that is, Hamiltonians on these vector spaces $\mathcal{H}_V$. If A_i are operators (or matrices) on $\mathcal{H}_i$, operator monomials on $\mathcal{H}_V$ are given by

$$\bigotimes_{x_i} A_i \ : \bigotimes v_i \mapsto \bigotimes A_i \circ v_i \tag{6}$$

and (multi)linearly extended on more general vectors. Refraining from a too abstract approach we restrict ourselves to Hamiltonians given by a sum

over *one-point, two-point,..., k-point-interactions.* This means

$$\sum_{x_i} \Phi^1(x_i)\,,\ \sum_{x_i,x_j} \Phi^2(x_i,x_j)\,,\ \ldots \tag{7}$$

where

$$\Phi^1(x_i) = A_i^{(1)}\ ,\ \Phi^2(x_i,x_j) = A_i^{(2)} \otimes A_j^{(2)}\ ,\ \ldots \tag{8}$$

Assumption 2.1 *To avoid unneccessary complications we assume that only interaction terms up to a certain finite order occur in the Hamiltonian and that all the occurring operators A_i are hermitean.*

Remark: An operator like e.g. $A_i \otimes A_j$ or for short, A_iA_j operates on the full tensor product $\mathcal{H}_V$ by inserting the unit operator $\mathbf{1}$ for the remaining entries, i.e.

$$A_i \otimes A_j = \mathbf{1} \otimes \cdots \otimes A_i \otimes \mathbf{1} \otimes \cdots \otimes A_j \otimes \cdots \tag{9}$$

Obviously, all the A_i, A_j do commute for $i \neq j$. Therefore the interaction terms defined above are also hermitean as is their sum

Typical examples are spin systems, e.g.

$$H = \sum_i \overrightarrow{\sigma}_i \otimes \overrightarrow{\sigma}_{(i+1)} =: \sum_i \overrightarrow{\sigma}_i \overrightarrow{\sigma}_{(i+1)} \tag{10}$$

with σ denoting the usual Pauli-matrices and extension to higher dimensions being straightforward.

Usually one makes the assumption that the interaction has a *finite range* and is *translation invariant.*

Definition 2.2 *The interaction is called translation invariant if with $\Phi^k(x_{i_1},\ldots,x_{i_k})$ also $\Phi^k(x_{i_1}+r,\ldots,x_{i_k}+r)$ occurs in the Hamiltonian with r some lattice vector and both being the same operators.*

Definition 2.3 *The interaction is called to have a finite range, δ, if with one lattice point fixed, e.g. x_{i_1}, only finitely many members $\Phi^k(x_{i_1},y_{i_2},\ldots,y_{i_k})$ different from zero exist in H when the y_{i_l} vary over $\mathbb{Z}_a^d$, all y_j having a distance from x_i which is $\leq \delta$.*

In our above simple example only so-called *nearest-neighbor interactions* (nn) occur.

Remark: While we give these details for consistency reasons, only the general properties of such Hamiltonians will be of relevance in the following. So there is at the moment no need to go further into the details of all the model systems which fall in this class. Only their translation invariance and the finite range will be of some importance. More properly, it makes the analysis more transparent, while our results should hold also in a more general context.

What will be of interest for the following discussion is the restriction of a general Hamiltonian, H, to a certain subvolume $V \subset \mathbb{Z}_a^d$.

Definition 2.4 *The restriction of a general Hamiltonian, H, of the kind described above to a subvolume $V \subset \mathbb{Z}_a^d$ is the operator H_V which consists of all the interaction terms which lie in V, i.e., only k-tuples $(x_{i_1}, \ldots, x_{i_k})$ are admitted with all the $x_{i_l} \in V$.*

$$H_V := \sum_{k; x_{i_l} \in V} \Phi^k(x_{i_1}, \ldots, x_{i_k}) =: \sum_{n(V)} \Phi^k \tag{11}$$

($n(V)$, the number of terms in the sum being of order $O(|V|)$).

Another important part of the total H relative to a given volume V is the *boundary contribution* H_V^{bd}.

Definition 2.5 *By H_V^{bd} we denote the part of the total H which consists of all interaction terms which have both lattice points in V and the dual set $V' := \mathbb{Z}_a^d \setminus V$.*

$$H_V^{bd} := \sum_{k; x \in V, y \in V'} \Phi^k(x_{i_1}, \ldots; y_{i_l}, \ldots, y_{i_k}) \tag{12}$$

Observation 2.6 *It will be important in the following that with the Hamiltonian having finite range and $k \leq K$, the number of terms in H_V^{bd} is of order (area of boundary of V). We denote this number of terms by $n(V, V')$.*

We can make more detailed statements if we concentrate on the large subclass of models with all the Φ^k bounded operators (which holds for example if all the $\mathcal{H}_i$ are finite dimensional). This together with the assumed translation invariance and the above observation allow us to make the following important estimates.

Proposition 2.7 *Under the preceding assumptions we have*

$$\| H_V \| \leq C \cdot n(V) \ , \ \| H_V^{bd} \| \leq C' \cdot n(V, V') \tag{13}$$

where in the generic case, which we usually assume to prevail, both norms are actually proportional to the volume, the area of the boundary, respectively.
In case the local Hilbert spaces $\mathcal{H}_i$ are finite dimensional, all the occurring Hamiltonians are large but nevertheless finite hermitean matrices for finite V, hence having a discrete spectrum with the number of eigenvalues (counting multiplicity) being the same as the dimension of the respective Hilbert spaces (the eigenvalues being the zeros of the characteristic polynomial).

It is obvious that this latter observation greatly simplifies the quantitative analysis.

As we will in the following mainly discuss the case where the local Hilbert spaces have finite dimension, some remarks are in order concerning the possible extension of our findings to the more general situation of infinite dimensional Hilbert spaces as e.g. the example of large arrays of coupled harmonic oscillators. For the time being we assume that the spectra of the local and global hamiltonians are discrete but are now *not* necessarily bounded from above. We still assume that H_V is bounded from below (existence of a groundstate!).

So let H be such a Hamiltonian on a separable Hilbert space, $\mathcal{H}$. We select a certain (countable) basis, e_i, and choose certain subspaces, $\mathcal{H}_n$, spanned by the basis vectors, $e_1, \ldots, e_n$. The projector on $\mathcal{H}_n$ is denoted by P_n. Then

$$P_n \cdot H \cdot P_n \tag{14}$$

is a bounded operator on $\mathcal{H}_n$. Being a little bit more general, if H_V is the Hamiltonian on $\mathcal{H}_V := \mathcal{H}_{i_1} \otimes \cdots \otimes \mathcal{H}_{i_N}$, we select in each $\mathcal{H}_{i_\nu}$ the subspace $\mathcal{H}_i^{(n)}$, spanned by $e_1^{(i)}, \ldots, e_n^{(i)}$. From these local pieces we compose the subspace, $\mathcal{H}_n$, in $\mathcal{H}_V$, i.e.

$$\mathcal{H}_n := \mathcal{H}_{i_1}^{(n)} \otimes \cdots \otimes \mathcal{H}_{iN}^{(n)} \tag{15}$$

and denote again the projector on this subspace by P_n. In the same manner we take

$$H^{(n)} := P_n \cdot H_V \cdot P_n \tag{16}$$

as finite dimensional Hamiltonian on these $\mathcal{H}_n \subset \mathcal{H}_V$.

Now we have to discuss what happens if we take the limits

$$\mathcal{H}_n \to \mathcal{H}_V \ , \ H^{(n)} \to H_V \quad \text{etc.} \tag{17}$$

Note that by construction all the $H^{(n)}$ are now bounded, even finite dimensional, but the limit Hamiltonians are in general unbounded. We do not want to be too tedious concerning technical details of functional analysis at this point. Suffice it to say that a reasonable concept of operator convergence in this context is convergence in the *resolvent sense*, i.e., instead of dealing with unbounded operators we deal with their bounded resolvents

$$(H - z)^{-1} \ , \ \mathrm{Im}(z) \neq 0 \tag{18}$$

Under quite weak assumptions, which are in general fulfilled in our context, (strong) resolvent convergence can be assumed (cf. [11], sect. VIII.7). As a consequence we have the following result (discrete spectrum):

Observation 2.8 *With H having discrete spectrum and if $H_n \to H$ in strong resolvent sense, we can find to each eigenvalue E of H an interval (a, b) so that E is the only spectral value of H in (a, b). With $P^{(n)}_{(a,b)}$ the spectral projections of H_n on the interval (a, b) we have*

$$P^{(n)}_{(a,b)}\psi \to P_{(a,b)}\psi = P_E\psi \tag{19}$$

for all $\psi \in \mathcal{H}$. We get even stronger results if we assume convergence in norm-resolvent sense.

We now sketch how results about entanglement-entropy, derived for large but nevertheless finite dimensional systems, could be transferred to the general case. But as there are several quite delicate technical steps involved, which to rigorously prove would need quite an amount of mathematical input, we refrain from giving all the intricate mathematical details at the moment. From a physical point of view the strategy seems to be quite reasonable.

In a first step we have to guarantee that for example in the case of groundstates

$$\Psi^{(n)}_0 \to \Psi_0 \tag{20}$$

In the following sections we regard these vectorstates as states on a restricted region, V_1, and the corresponding Hilbert space or observable algebra. We then have for the respective density matrices over $\mathcal{H}_1$

$$W^{(n)}_1 \to W_1 \tag{21}$$

in the form

$$Tr(W_1^{(n)} \cdot A) \to Tr(W_1 \cdot A) \tag{22}$$

What we need is a result like

$$W_1^{(n)} \cdot \ln W_1^{(n)} \to W_1 \cdot \ln W_1 \tag{23}$$

in a suitable topology so that we may get in the end

$$Tr(W_1^{(n)} \cdot \ln W_1^{(n)}) \to Tr(W_1 \cdot \ln W_1) \tag{24}$$

that is

$$S(W_1^{(n)}) \to S(W_1) \tag{25}$$

Remark: Some of the necessary technical arsenal can be found for example in [12].

3 Some General Remarks on Partial Trace and Entanglement Entropy

Let us take a vector state, Φ, from the Hilbert space $\mathcal{H}_V$ with V large (or macroscopic). Let us divide V into $V_1 \cup V_2$ and take the respective Hilbert spaces, $\mathcal{H}_1, \mathcal{H}_2$. As both $\mathcal{H}_V$ and the operator algebra of bounded operators over $\mathcal{H}_V$ is of tensorial character, we have

$$\mathcal{H}_V = \mathcal{H}_1 \otimes \mathcal{H}_2 \ , \ \mathcal{A}_V = \mathcal{A}_1 \otimes \mathcal{A}_2 \tag{26}$$

where each operator in $\mathcal{H}_V$ can e.g. be written as a sum over elementary generators of the following kind. With $|e_i>$, $|e'_j>$ bases in $\mathcal{H}_1, \mathcal{H}_2$ respectively, we construct the generators

$$|e_i >< e_l| \otimes |e'_j >< e'_m| \tag{27}$$

which map, for example $|e_l> \otimes |e'_m> \to |e_i> \otimes |e'_j>$. $\mathcal{A}_1$, $\mathcal{A}_2$ are embedded in $\mathcal{A}_V$ via

$$\mathcal{A}_1 \to \mathcal{A}_1 \otimes \mathbf{1} \, , \, \mathcal{A}_2 \to \mathbf{1} \otimes \mathcal{A}_2 \tag{28}$$

Thus we can evaluate the pure state, Φ on the restrictions $\mathcal{H}_1, \mathcal{H}_2$ via

$$\omega_1(A^{(1)}) := (\Phi|(A^{(1)} \otimes \mathbf{1})\Phi) \, , \, \omega_2(B^{(2)}) := (\Phi|(\mathbf{1} \otimes B^{(2)})\Phi) \tag{29}$$

thus defining the states ω_1 , ω_2 on $\mathcal{H}_1, \mathcal{H}_2$. Choosing a basis $e_i \otimes e'_j$ in the tensor product $\mathcal{H}_V = \mathcal{H}_1 \otimes \mathcal{H}_2$ we get

$$\Phi = \sum c_{ij} \, e_i \otimes e'_j \tag{30}$$

and

$$(\Phi|(A\otimes\mathbf{1})\Phi)=\sum_{m,i,j}\overline{c}_{im}c_{jm}(e_i|Ae_j)=\sum_{i,j}b_{ij}(e_i|Ae_j) \tag{31}$$

with

$$b_{ij}=\sum_{m=1}^{dim(\mathcal{H}_2)}\overline{c}_{im}c_{jm} \tag{32}$$

This can be rewritten as

$$\omega_1(A)=Tr(W_1\cdot A)\quad\text{with}\quad W_1:=\sum_{ij}b_{ij}|e_j><e_i| \tag{33}$$

Viewing the matrices $C:=(c_{jm})_{mj}$, $C^*:=(\overline{c}_{im})_{im}$ as operators from $\mathcal{H}_1\to\mathcal{H}_2$, $\mathcal{H}_2\to\mathcal{H}_1$ respectively, we have

$$W_1=C^*\cdot C\ ,\ W_2=C\cdot C^* \tag{34}$$

where $(c_{jm})_{mj}$ means, the coefficient c_{jm} occupies the position (mj) in the matrix with j labelling the $\mathcal{H}_1$-basis, m the $\mathcal{H}_2$-basis. If ψ_i is an eigenvector of $W_1=C^*\cdot C$, i.e.

$$C^*\cdot C\circ\psi_i=\lambda_i\cdot\psi_i \tag{35}$$

it follows that

$$CC^*C\circ\psi_i=\lambda_i\cdot C\circ\psi \tag{36}$$

i.e., λ_i is eigenvalue of $W_2=CC^*$ with eigenvector $C\psi_i$ and vice versa. Furthermore, if $\lambda_i\neq 0$, the degeneracy is the same with respect to C^*C and CC^*. This follows from

$$(C\psi_i^1|C\psi_i^2)=(\psi_i^1|C^*C\psi_i^2)=\lambda_i(\psi_i^1|\psi_i^2) \tag{37}$$

that is, with ψ_i^1 , ψ_i^2 orthogonal eigenvectors to the eigenvalue $\lambda_i\neq 0$, $C\psi_i^1$, $C\psi_i^2$ are also orthogonal and non-vanishing and the same holds in the other direction.

By the same token we infer from the positive definiteness of C^*C and CC^* that all eigenvalues are ≥ 0. The normalisation of the vector Φ as a state on $\mathcal{A}$ and $\mathcal{A}_i$ implies that the trace norm of W_i is one. We hence have

Theorem 3.1 *The partial traces W_1 , W_2 have the same spectrum and the eigenvalues $\neq 0$ have the same multiplicity while the respective zero-eigenvalues may have different degeneracies, depending on the in general different dimensions of $\mathcal{H}_1$, $\mathcal{H}_2$.*

Corollary 3.2 *The (entanglement-)entropies of the states* ω_1 , ω_2 *or* W_1 , W_2 *are the same, i.e.*

$$S_2(W_2) = S_1(W_1) := -\sum \lambda_i \cdot \ln \lambda_i \tag{38}$$

Remark: Note that the dimensions of $\mathcal{H}_1$, $\mathcal{H}_2$ can be very different. This already shows that *entanglement-entropy* cannot have in general an ordinary linear volume-dependence as in our context small or large Hilbert spaces are connected with small or large volumes.

On the other hand we know that the usual thermodynamic entropy is an extensive quantity and depends in general linearly on the volume. So let us assume we have a Gibbs-state on the volume V_1 with Hamiltonian H_1, its eigenvalues and eigenstates being E_i , ψ_i. That means:

$$\omega_1(A) := Tr(e^{-\beta H_1} \cdot A)/Tr(e^{-\beta H_1}) \tag{39}$$

with β the inverse temperature $1/kT$. It follows

$$S_1 = -\sum p_i \ln p_i \ , \ p_i = e^{-\beta E_i}/\sum e^{-\beta E_i} \tag{40}$$

and

$$S_1(V_1) \sim V_1 \tag{41}$$

We now adjoin a volume V_2 with a Hilbert space $\mathcal{H}_2$ of sufficiently high dimension. We define the following vector, Ψ, in $\mathcal{H}_1 \otimes \mathcal{H}_2$.

$$\Psi := \sum \sqrt{p_i}\, \psi_i \otimes e_i \tag{42}$$

(e_i spanning a basis in $\mathcal{H}_2$ and degeneracies being included). We have

$$(\Psi | A^{(1)} \Psi) = Tr(e^{-\beta H_1} \cdot A^{(1)})/Tr(e^{-\beta H_1}) \tag{43}$$

We conclude:

Observation 3.3 *Every Gibbs state over* $\mathcal{A}_1$ *can be represented by a vector state in a sufficiently large ambient Hilbert space. Restricted to* $\mathcal{H}_1$ *this vector state is the partial trace, but we see from our above reasoning that the entanglement-entropy of* Ψ *relative to* V_1 *is now proportional to the volume* V_1.

It is important for the physical understanding and intuition to get a better feeling how entanglement-entropy is affected in both a quantitative and qualitative way by varying physical conditions. We remember in this connection the various ensembles in statistical mechanics and their quantitative or, at least, qualitative similar macroscopic properties under a wide range of conditions. It is perhaps particularly useful to introduce concepts which are, at least in a rough sense, of a similar character as entanglement-entropy because the latter can only be calculated in very few special cases. We think in this context of the relation between, for example, the canonical and the microcanonical ensemble in statistical mechanics.

For one, it is obvious that the entropy of a state, ψ_0, reduced to, say, V_1 or V_2, does not depend on the choice of Hilbert space bases in the corresponding Hilbert spaces. So, in the following, we will frequently subdivide V_1 or V_2 further into, say, $V_1 = V_1' \cup V_1''$ with V_1'' a boundary layer in V_1 neighboring upon the interface, separating V_1 and V_2. One can then equally well choose a basis in $\mathcal{H}_1$ by forming the tensor product of the respective bases in $\mathcal{H}_1'$ and $\mathcal{H}_1''$ etc.

For another, a famous theorem of E.Schmidt and von Neumann ([13],[14]) states that Ψ_0 in $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be represented in the special form

$$\Psi_0 = \sum_i \sqrt{\lambda_i} \cdot \phi_{i,1} \otimes \phi_{i,2} \tag{44}$$

with $\phi_{i,1}$, $\phi_{i,2}$ particular orthonormal bases in $\mathcal{H}_1$, $\mathcal{H}_2$ (the so-called Schmidt-basis; this was also exploited in [15]).

Remark: In modern parlance this is nothing but the theorem that a compact operator can be put into such a canonical spectral form. Note in this context that Ψ_0, viewed as an operator from $\mathcal{H}_2$ to $\mathcal{H}_1$, belongs to the *Hilbert-Schmidt-class* as a consequence of its normalisation as a vector.

Ψ_0 reduced to $\mathcal{H}_1$ then yields:

$$(\Psi_0|A^{(1)}\Psi_0) = \sum_i \lambda_i \cdot (\phi_{i,1}|A\phi_{i,1}) = Tr(W_1 \cdot A) \tag{45}$$

What is important in this particular representation is that both systems of vectors are orthonormal. With $\Phi = \sum_{ij} c_{ij} e_i \otimes e_j'$ we can of course always write

$$\Phi = \sum_i e_i \otimes \phi_i = \sum_j \psi_j \otimes e_j' \tag{46}$$

with

$$\phi_i = \sum_j c_{ij}\, e'_j \ , \ \psi_j = \sum_i c_{ij}\, e_i \tag{47}$$

The reduction to $\mathcal{H}_1$, $\mathcal{H}_2$ then yields:

$$(\Phi|A^{(1)}\Phi) = \sum_j (\psi_j|A\psi_j) \ , \ (\Phi|B^{(2)}\Phi) = \sum_i (\phi_i|B\phi_i) \tag{48}$$

Trying to relate the canonical version of the notion of entropy, $S(W) := -\sum_i p_i \ln p_i$ with some other (perhaps coarser) concept, and acknowledging the fact that in general it is out of question to really calculate the eigenvalues, p_i, of the density matrix belonging to the restriction of a complicated entangled state, one may be inspired by the beautiful analysis of the entropy concept, as it is laid out in [16], sect.7 of chapt.1. It is shown there that the natural quantity which should be relevant in this context is the number of microscopic quantum states, $\triangle\Lambda$, a macrostate is smeared over or, in other words, the number of microstates which essentially contribute in a macrostate (taken with equal weights). It is then shown in [16] that in the regime of equilibrium statistical mechanics, the logarithm of this quantity coincides with the canonical notion of entropy given above, but this result is far from trivial. We see that $\ln \triangle\Lambda$, giving equal apriori weight to the members of a certain selected sample of quantum states, implements the philosophy of the microscopic ensemble picture.

Remark: One should note that the simplicity of the canonical formula for the entropy is only apparent. Even if one happens to know the Boltzmann weights, what is equally important is the local *density of states* for macroscopic quantum systems. This is generally unknown for large interacting systems.

In the following sections we are primarily interested in estimates of the kind "order of", that is, estimates of quantities on a scale given by e.g. a certain volume or by the area of some bounding surface etc., and this typically only on a logarithmic scale. That is, we are at the moment not really interested in detailed quantitative results. So, inspecting the above formulas, we see that a rough notion which reflects somehow the number of "different" states being involved in the reduction of a vector state to a certain subvolume is the dimension of the Hilbert subspace the contributing vectors are lying in. This however needs more qualifications.

In a first step we regard the above representation of the vector Φ as a map from the Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$ to the corresponding subspaces spanned by

the ϕ_i , ψ_j, respectively. This map is given by $C = (c_{ij})$ and the transposed matrix. From linear algebra we know that the dimension of these subspaces is given by the rank of the matrices C, C^T, with the ranks of C and its transpose C^T being equal. Viewing C as an abstract map on $\mathcal{H}_2$, it is obvious that this dimension cannot depend on the chosen basis. We hence have

Observation/Definition 3.4 *The dimension of the subspaces, spanned by ϕ_i or ψ_j as image vectors under the maps C , C^T applied to certain bases are equal and independent of the chosen bases in $\mathcal{H}_1$, $\mathcal{H}_2$. Furthermore its logarithm represents a certain measure of the entanglement entropy on the scale "order of" under certain favorable conditions. These conditions may be: All image vectors contribute with roughly the same strength, or, rather, their respective weights are not too different. Or, some of the matrix elements happen to be very small compared with the rest so that one can go over to a purified matrix; in particular, some of the image vectors may be very small and can be neglected. In these cases one will get some approximation of the original entanglement-entropy.*

In the following sections we will apply this approximative concept of entanglement-entropy.

4 Perturbation of Hamiltonians

The preceding section shows clearly that the details of the dependence of (entanglement-)entropy on volume and/or area are presumably subtle and intricate and need more qualifications. This holds the more so if one wants to treat this problem on a broad scale , that means, if one wants to discuss whole classes of models. We learned in particular that the vector state we start from has to be characterized more properly.

So we start from a Hilbert space, $\mathcal{H}_V$, over a macroscopic volume V and divide it into two connected subvolumes, $V = V_1 \cup V_2$, both V_1 , V_2 still being macroscopic with

$$\mathcal{H}_V = \mathcal{H}_1 \otimes \mathcal{H}_2 \tag{49}$$

We assume a Hamiltonian, H_V, to be given on $\mathcal{H}_V$ of the kind described above. This Hamiltonian can be written as

$$H_V = H_{V_1} + H_{V_2} + H_{bd} \tag{50}$$

with $H_{V_i} =: H_i$ (in the following) the commuting Hamiltonians of the regions V_1 , V_2 and H_{bd} denoting the part of the interaction which comprises lattice

points of both V_1 and V_2. That is, we have

$$[H_1, H_2] = 0 \ , \ [H_i, H_{bd}] \neq 0 \tag{51}$$

It sometimes happens that we have to discriminate between, for example, H_1 restricted to the subspace $\mathcal{H}_1$ and its embedded version, acting on the full Hilbert space by tensoring with the unit operator of the volume V_2.

Definition 4.1 *We denote the embedded operators by H_1 etc. and the restricted versions by H_1^r etc.*

Generically H_i are of "size" V_i (e.g. their respective operator norms or (most of their) eigenvalues). That is

$$\parallel H_i \parallel \leq C_i \cdot n(V_i) = O(V_i) \ , \ \parallel H_{bd} \parallel \leq C' \cdot n(V_1, V_2) = O(boundary_{1,2}) \tag{52}$$

Therefore one may have the idea to treat H_{bd} as a relatively small perturbation of the operators H_1 or H_2.

The operators H_1 , H_2, defined above over the regions V_1 , V_2, commute. In the following we will encounter in various arguments such pieces of the total Hamiltonian which commute. Another example is the following. We subdivide V_1 further into regions V_1' , V_1'' and correspondingly for V_2 with $V_1 = V_1' \cup V_1'$. V_1'' is the region in V_1 which lies within distance $d \geq \delta$ (δ the maximum over the ranges of the various interaction potentials) of the common boundary with V_2. In certain calculations we choose d macroscopic but $L \gg d \gg \delta$ (where, as usual, we take δ as a microscopic quantity). The respective Hilbert spaces are $\mathcal{H}_1'$, $\mathcal{H}_1''$ with $\mathcal{H}_1 = \mathcal{H}_1' \otimes \mathcal{H}_1''$. We can now define another approximation of the total Hamiltonian H in deleting the boundary terms with respect to the interfaces separating V_1' , V_1'' on the one hand and V_2' , V_2'' on the other hand,

$$H' := H_1' + H_1'' + H_{bd} + H_2' + H_2'' =: H_1' + H_{bd}' + H_2' \tag{53}$$

with

$$H_{bd}' := H_1'' + H_{bd} + H_2'' \tag{54}$$

We now have

Observation 4.2 *The operators H_1' , H_{bd}' , H_2' commute and*

$$H = H' + H_{bd(1)} + H_{bd(2)} \tag{55}$$

with the two boundary contributions describing the interaction through the interfaces between V_1' , V_1'' and V_2' , V_2''. The advantage is that we now still have included the interaction through the common interface between V_1 , V_2 in H', the interface we are originally interested in.

As to such commuting operators we have the following spectral result (cf. e.g. [18] or [21]) which goes back to v.Neumann.

Theorem 4.3 *With (for simplicity reasons) $H_1, H_2, \ldots$ commuting bounded selfadjoint operators, they all are functions of a common selfadjoint operator, A, i.e. $H_i = f_i(A)$. It follows in particular that, in case the spectra are discrete, it exists a complete set of common eigenvectors for this set of commuting Hamiltonians (including multiplicities).*

One problem which however arises immediately if one wants to apply perturbation theory of operators is the following (if one is not entirely cavalier as to mathematical rigor). We know from almost every discussion of the foundations of statistical mechanics that for macroscopic volumes the spectrum of, say, the corresponding Hamiltonians, while being frequently discrete, is nevertheless so extremely dense and/or highly degenerate that ordinary perturbation theory is practically useless. A rough estimate yields the following qualitative results. The number of eigenvalues (counting degeneracy) of a hermitean matrix is the same as the dimension of the underlying Hilbert space. This means in our case

$$\#(eigenvalues\ of\ H_V) = D^{N_V} \tag{56}$$

(D the dimension of the local Hilbert spaces $\mathcal{H}_{x_i}$, N_V the number of sites in V). On the other hand, the spectrum of the corresponding Hamiltonian extends typically over an interval of order $|V|$.

That is, whereas the higher excited states are typically much more degenerate and the spectrum is certainly not evenly distributed, a very crude estimate yields a typical *density of states* of the order $O(|V|^{-1} \cdot D^{|V|})$. This prevents the immediate and naive application of ordinary (analytic) perturbation theory, which works well for perturbations small compared to the distance of neigboring eigenvalues of the unperturbed Hamiltonian. To be more precise, one knows (from results derived by Rellich), and in particular for the finite dimensional case, that for hermitean perturbations the (discrete) eigenvalues and eigenstates are *real-holomorphic* in the coupling constant not only for very small values (see for example [17], [21] or [19]).

Theorem 4.4 *With $H_\varepsilon := H_0 + \varepsilon V$ selfadjoint for $\varepsilon \in \mathbb{R}$, $H_0\,, V$ bounded (for simplicity reasons) and H_ε having purely discrete spectrum, the eigenvalues $\lambda_i(\varepsilon)$ and eigenvectors $\psi_i(\varepsilon)$ of H_ε, with $\lambda_i(0)\,, \psi_i(0)$ the eigenvalues and eigenvectors of H_0, are real analytic functions of ε. One can in particular choose $\varepsilon = 1$. It can however happen that eigenvalues cross (and hence degeneracies change in a superficial sense; see the following corollary).*

Corollary 4.5 *This implies that multiplicities belonging to a fixed $\lambda_i(\varepsilon)$ can only change at $\varepsilon = 0$ as analytic functions, being identical on a certain interval, are necessarily the same everywhere. The other ε-values where a singular behavior can occur lie in the complex plane away from the real axis. Note however that, as the eigenvalue functions can cross at some points, the counting of degeneracies at such points is a matter of taste. The dimension of the total eigenspace is of course the dimension of the union of the individual eigenspaces belonging to the different $\lambda_i(\varepsilon)$ which meet at that point.*

On the other hand, convergence radii of the corresponding local power series expansions happen to be of the order of the distances between the points of the spectrum. This prevents to some extent concrete quantitative estimates. To see more clearly the true nature of the problem, we would, for example, like to start from the unperturbed groundstate, $\Psi_0^{(0)}$, of $H^{(0)} := H_1 + H_2$ and try to infer with the help of perturbation theory the structure of the corresponding groundstate Ψ_0 of $H^{(0)} + H_{bd}$ as a power series expansion with respect to the eigenvectors of $H^{(0)}$. That is,

$$\Psi_0 = \sum c_m \cdot \Psi_m^{(0)} \tag{57}$$

with

$$c_m = c_m^{(0)} + c_m^{(1)} + \dots \ , \ c_0^{(0)} = 1 \, , \, c_m^{(0)} = 0 \text{ for } m \neq 0 \tag{58}$$

The first order yields

$$c_m^{(1)} = V_{m0}/(E_m^{(0)} - E_0^{(0)}) \ , \ m \neq 0 \, , \quad \text{and} \quad V_{m0} = (\Psi_m^{(0)} | V \cdot \Psi_0^{(0)}) \tag{59}$$

We see that for perturbation theory to make sense,

$$|V_{m0}| < |E_m^{(0)} - E_0^{(0)}| \tag{60}$$

In more general terms, with $H = H_0 + V$ and V the perturbation, most of rigorous perturbation theory is based on the following representation of the resolvent of H:

$$(H - E)^{-1} = (H_0 - E)^{-1} \cdot (\mathbf{1} + V/(H_0 - E))^{-1} \tag{61}$$

Frome this one can for example infer that with E not an eigenvalue of H_0 (i.e. lying in the so-called *resolvent set*), it is also not an eigenvalue of H provided that $\| \, V/(H_0 - E) \, \| < 1$. We have the estimate

$$\| \, V/(H_0 - E) \, \| \leq \| \, V \, \| \cdot \| \, (H_0 - E)^{-1} \, \| \tag{62}$$

and as

$$(H_0 - E)^{-1} = \int (E' - E)^{-1} dP(E') \tag{63}$$

$\| (H_0 - E)^{-1} \|$ becomes large if the distances between the points of the spectrum of H_0 are small.

Observation 4.6 *While H_{bd} is much smaller than H_1 or H_2 in general, it is still a macroscopic perturbation compared to the typically microscopic distances between the eigenvalues of H_i. So ordinary perturbation theory is not immediately applicable.*

Remark: There exists however a (complicated and tedeous) way to deal with such problems to a certain extent (at least in the physics literature; see the remarks at the end of the last two sections or e.g. [20]).

What will however better work is another important method of estimating eigenvalues and their changes under perturbations which does not focus so much on the motion of individual eigenvalues under a perturbation but rather makes more global and qualitative statements. This method provides however no information about the respective eigenvectors, our main point of interest. The method is based on the so-called *Rayleigh-Ritz-principle* and/or the *Poincare-Courant-Weyl estimates* (cf. for example [21] or [22]). All these statements are based on *minimum-maximum- or maximum-minimum-estimates* together with the principle of stronger or weaker constraints on sets of comparison Hilbert space vectors.

A result, useful in our context, can e.g. be found in [21], p.224, that is, the so-called Weyl-Courant-inequalities, which we reformulate here for bounded hermitean operators with discrete and only finitely degenerated spectrum (not having zero as an accumulation point).

Remark: For various reasons the numbering of eigenvalues is different in [21]. We start the counting, beginning with the groundstate.

Theorem 4.7 *With A_1, A_2 operators of the above kind, with sets of eigenvalues, chosen in increasing order (counting multiplicity),*

$$E_0^1 \leq E_1^1 \leq \ldots \; ; \; E_0^2 \leq E_1^2 \leq \ldots \tag{64}$$

and

$$E_0 \leq E_1 \leq \ldots \tag{65}$$

the corresponding eigenvalues of $A := A_1 + A_2$, we have the estimates

$$E_{p+q} \geq E_p^1 + E_q^2 \; , \; p, q = 0, 1, 2, \ldots \tag{66}$$

Corollary 4.8 *With $H = H_0 + V$ and V a small perturbation of H_0, we have*

$$E_0^1 - \parallel V \parallel \leq E_0 \leq E_0^1 + \parallel V \parallel \tag{67}$$

and more generally

$$E_p^1 - \parallel V \parallel \leq E_p \leq E_p^1 + \parallel V \parallel \tag{68}$$

E_0, E_0^1 the groundstates of H, H_0 respectively.

Proof: The lhs of the inequalities follows directly from the theorem and $|E_q^2| \leq \parallel V \parallel$ for all the eigenvalues of $V = A_2$. The rhs follows from the theorem by interchanging the roles of the operators, that is

$$A_1 = A - A_2 \tag{69}$$

and hence

$$E_{p+q}^1 \geq E_p + E_q(-A_2) \geq E_p - \parallel A_2 \parallel \tag{70}$$

i.e.

$$E_p \leq E_{p+q}^1 + \parallel A_2 \parallel \tag{71}$$

which yields the result by choosing $q = 0$. □

5 The Groundstate of the Hamiltonian

We begin with the calculation of the entanglement-entropy of the ground state, Ψ_0 of the full Hamiltonian over $V = V_1 \cup V_2$. In a first step we study the entanglement-entropy of the ground state, Ψ_0', of the approximate Hamiltonian, H', introduced in the preceding section. We saw that H' can be written as

$$H' = H_1' + H_2' + H_{bd}' \tag{72}$$

with all the terms on the rhs commuting with each other. Assuming again that the ground states are not degenerate we infer from the results of the previous section that the ground state energy, E_0', of H' can be uniquely written as

$$E_0' = E_{0,1}' + E_{0,2}' + E_{0,bd}' \tag{73}$$

with the rhs the sum of the ground state energies of the terms occurring on the rhs of the previous equation.

Remark: Note that the embedded Hamiltonians always have full subspaces, belonging to an eigenvalue. For example, H_1' has the eigenspace $\psi_{0,1}' \otimes \mathcal{H}_1''$

belonging to the ground state energy $E'_{0,1}$ in the Hilbert space $\mathcal{H}_1 = \mathcal{H}'_1 \otimes \mathcal{H}''_1$ and $\psi'_{0,1}$ the unique ground state of the restricted $H'_{1,(r)}$ acting on $\mathcal{H}'_1$.

The need to constantly make these distinctions is a bit nasty and we will be a little bit sloppy if no confusion can arise. We then have

Observation 5.1 *The ground state, Ψ'_0 of H' can now be uniquely represented as the tensor product of the ground states of the restricted Hamiltonians, i.e.*

$$\Psi'_0 = \psi'_{0,1} \otimes \psi'_{0,2} \otimes \psi'_{0,bd} \tag{74}$$

where

$$\psi'_{0,bd} \in \mathcal{H}''_1 \otimes \mathcal{H}''_2 \tag{75}$$

In order to calculate the partial traces with respect to $\mathcal{H}_1$ or $\mathcal{H}_2$ we have in a first step to develop Ψ'_0 with respect to a basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ or, what amounts to the same, $\mathcal{H}'_1 \otimes \mathcal{H}''_1 \otimes \mathcal{H}'_2 \otimes \mathcal{H}''_2$. Choosing as bases in the subspaces the eigenvectors of the restricted Hamiltonians $H'_{1,(r)}$, $H'_{2,(r)}$, $H''_{1,(r)}$, $H''_{2,(r)}$, we can infer the following from the above observation.

Conclusion 5.2 *In the representation of Ψ'_0 with respect to the mentioned basis in*

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}'_1 \otimes \mathcal{H}''_1 \otimes \mathcal{H}''_2 \otimes \mathcal{H}'_2 \tag{76}$$

the outermost left and right terms on the rhs remain fixed (no summation). The only summation occurs in the boundary term, $\psi'_{0,bd}$, which is developed with respect to a basis in $\mathcal{H}''_1 \otimes \mathcal{H}''_2$. Taking for example the eigenvectors of $H''_{1,(r)}$, $H''_{2,(r)}$ we write

$$\psi'_{0,bd} = \sum c'_{i,j}\, \psi''_{i,1} \otimes \psi''_{j,2} \tag{77}$$

and

$$\Psi'_0 = \psi'_{0,1} \otimes (\sum \ldots) \otimes \psi'_{0,2} \tag{78}$$

We have

$$H'_{bd} = H''_1 + H''_2 + H_{bd} \tag{79}$$

where the operators occurring on the rhs are all of roughly the same size, i.e. of order $O(boundary_{1,2})$. While H''_1 , H''_2 commute, the support of H_{bd} overlaps both with the support of H''_1 and H''_2 and the respective commutators are typically quite different from zero.

If we now view Ψ'_0 as a state over $\mathcal{A}^1$, the algebra on $\mathcal{H}_1 = \mathcal{H}'_1 \otimes \mathcal{H}''_1$ we get:

$$(\Psi'_0|(A \otimes \mathbf{1})\Psi'_0) = (\psi'_{0,1} \otimes \psi'_{0,bd}|(A \otimes \mathbf{1})\psi'_{0,1} \otimes \psi'_{0,bd}) \tag{80}$$

where on the lhs $\mathbf{1}$ is the unit operator on $\mathcal{H}_2$, on the rhs it is the unit operator on $\mathcal{H}''_2$. Inserting $\psi'_{0,bd} = \sum c'_{i,j}\, \psi''_{i,1} \otimes \psi''_{j,2}$ in the above expression we get

$$\begin{aligned}(\Psi'_0|(A \otimes \mathbf{1})\Psi'_0) &= \sum_{ij} \sum_{l} \overline{c}'_{il} c'_{jl} (\psi'_{0,1} \otimes \psi''_{i,1}|A \circ \psi'_{0,1} \otimes \psi''_{j,1}) \\ &= \sum_{ij} b_{ij} (\psi'_{0,1} \otimes \psi''_{i,1}|A \circ \psi'_{0,1} \otimes \psi''_{j,1}) \end{aligned} \tag{81}$$

with $b_{ij} = \sum_l \overline{c}'_{il} c'_{jl}$.

Conclusion 5.3 *The reduced state or density matrix on $\mathcal{H}_1$, corresponding to the total vector state, Ψ'_0, is*

$$W'_1 = |\psi'_{0,1} >< \psi'_{0,1}| \otimes W''_1 \tag{82}$$

with W''_1 the density matrix on $\mathcal{H}''_1$ with matrix elements b_{ij}.

If the local Hilbert spaces have uniform dimension D and with the assumed finite interaction distance δ, we conclude that the dimension of the Hilbert space $\mathcal{H}''_1$ is of order $O(D^{|bd_{1,2}|})$. From the preceding conclusion we infer that for the vector Ψ'_0 all perturbations are essentially restricted to the boundary region.

Conclusion 5.4 *For sufficiently generic boundary Hamiltonians, H_{bd}, the groundstate of H' is expected to contain or is scattered over a number of eigenstates of H''_1 of the order $O(D^{|bd_{1,2}|})$. Correspondingly we infer that its entanglement-entropy in the generic case is of order $O(|bd_{1,2}|)$.*

Remark: The deeper reason why we are able to infer such a general result for the approximate Hamiltonian H' is, on the one hand, the sufficient localisation of the perturbation in a boundary layer of finite thickness and, on the other hand, the uniqueness properties of the groundstate as a tensor product of the corresponding groundstates of the Hamiltonians of the subvolumes.

Now we come to the groundstate of the full Hamiltonian

$$H = H' + H_{bd(1)} + H_{bd(2)} \tag{83}$$

The difference between H and H' is a small perturbation on the scale of H or H' as, say, operators, but not on the scale defined by the difference between neighboring eigenvalues of H , H'. From the preceding section we know at least that

$$E'_P - \triangle \leq E_p \leq E'_p + \triangle \tag{84}$$

with

$$\triangle = \| H_{bd(1)} + H_{bd(2)} \| = O(|bondary_{1,2}|) \tag{85}$$

Our plan is to make an inference from the number of eigenstates of $H'_1 + H''_1$ which essentially contribute in the representation of Ψ'_0 to the corresponding number which essentially contribute in the representation of Ψ_0, the groundstate of the full Hamiltonian. This number should be of the same order as the corresponding number of eigenstates of H_1, as both sets represent complete bases in $\mathcal{H}_1 = \mathcal{H}'_1 \otimes \mathcal{H}''_1$.

We do this in several steps using the following trick. In a first step we add the boundary interaction $H_{bd(2)}$ to the start Hamiltonian H' yielding the intermediate Hamiltonian $H'_1 + H(V''_1 \cup V_2)$. Its groundstate is $\psi'_{0,1} \otimes \phi'_0$ with ϕ'_0 the groundstate of $H(V''_1 \cup V_2)$. In V_1 we have more or less the same situation as before with possible perturbations again confined (by definition) to the region V''_1. The same argument as before yields an entropy for the reduced state over V_1 of order $O(|bd_{1,2}|)$. Now we employ the fact that the entropies are necessarily the same on both sides. That is, we arrive at

Observation 5.5 *The entropy of the state ϕ'_0 reduced to V_2 is of order $O(|bd_{1,2}|)$.*

Now we employ the localisation properties of $H_{bd(1)}$ about the interface bd_1 within a small strip of diameter 2δ, the interface itself having distance $d \gg \delta$ from the common boundary between V_1 and V_2. From general experience, drawn from the foundations of statistical mechanics and many-body-theory, we feel allowed to assume that deep inside the region V_2, i.e. in V'_2, the groundstate, Ψ_0, of the full Hamiltonian H should look similar to the groundstate, Φ'_0 of the Hamiltonian $H(V''_1 \cup V_2)$.

Remark: To be careful, we make the tacit assumption that our system is not in a *quantum-critical state*, i.e. correlations do not extend to infinity. The latter case would need some extra discussion.

Concerning the groundstate of the latter Hamiltonian we learned that its restriction to V_2 has an entropy of order $O(bd_{12})$. From the above we again conclude that, in V_2, Ψ_0 differs from Ψ'_0 (the groundstate of H') essentially

in a boundary layer about the interface bd_{12}. By symmetry we infer the same for the region V_1 and arrive at

Conclusion 5.6 *The above chain of reasoning leads to the conclusion that as a consequence of the spatial localisation properties of* H_{bd} , $H_{bd(1)}$, $H_{bd(2)}$ *and certain natural assumptions about clustering or decay of properties of influence and/or interactions, the groundstate of the full Hamiltonian,* H *, has an entanglement-entropy of order* $O(bd_{12})$*.*

6 The Higly Excited Eigenstates

To simplify the discussion we treat the following system. We take a huge box of sidelength L as the total volume V. We partition it by a lattice of small boxes, C_i, of sidelength l with $L \gg l \gg \delta$ (δ the range of the interaction in the original Hamiltonian, H. I.e., we assume that l is small but still macroscopic; this is the usual assumption in statistical mechanics. As subvolumes, V_1 , V_2 we take certain regions in V each of which contains an integer number of such small boxes. I.e., we assume (with N_l , $N_{l,1}$, $N_{l,2}$ the respective numbers of boxes in V , V_i)

$$N_l = N_{l,1} + N_{l,2} \ , \ N_l = L^3/l^3 \ , \ |V_i| = l^3 \cdot N_{l,i} \tag{86}$$

Each of the small boxes contains l^3/a^3 lattice sites of the original lattice. We assume of course that the interface, separating V_1 and V_2, is sufficiently regular, i.e. its area is assumed to be of order $O(L^2)$.

In each of the small boxes, C_i, we take as Hamiltonian, h_i, the piece of our original total Hamiltonian H, leaving out the interaction terms in H between the different boxes. Note that, due to the assumed translation invariance of our interaction, all the h_i are equivalent as operators. As these small boxes still contain quite a few lattice sites, the spectrum of $h = h_i$ may both be complex and degenerated. As new Hamiltonians on V , $V_{1,2}$ we take

$$H' := H'_V := \sum_V h_i \ , \ H'_{1,2} := \sum_{V_{1,2}} h_i \tag{87}$$

There is now, in contrast to the preceding section, no boundary term H_{bd}, operating in the vicinity of the boundary, bd_{12}, but the entanglement structure may still be quite complex as we will see below. But in contrast to the more general case it is better manageable.

Remark: Such systems are frequently discussed and their special properties

exploited in quantum statistical mechanics within the Gibbsian (ensemble) approach. See for example [23],[24],[25] or [26].

As all these h_i commute (by construction), the eigenstates and eigenvalues of H' or $H'_{1,2}$ can be built up from the more elementary components belonging to the h_i.

So, to begin with, let us start from some macroscopic volume, V', of the above kind ($V' = V$, $V_{1,2}$), the Hamiltonian, $H' = \sum_{V'} h_i$, and some eigenvalue, E, sufficiently far away from the groundstate energy $E_0 = \sum E_0^{(i)}$ with $E_j^{(i)}$ denoting the j-th energy level of the box Hamiltonian h_i. We have

$$E = \sum_{C_i} E_j^{(i)} \tag{88}$$

for certain combinations of energy levels, $E_j^{(i)}$, of the h_i.

The problem can now be phrased a little bit differently. With N boxes given and $h = h_i$ having the energy levels $E_1, E_2, \ldots, E_j, \ldots$, we are interested in the number of ways of distributing the energies, E_j, over the N boxes under the constraints

$$N = \sum N_j \quad , \quad E = \sum N_j \cdot E_j \tag{89}$$

with N_j the number of boxes having energy E_j. Each such configuration is hence characterized by the sequence, $(N_1, N_2, \ldots, N_j, \ldots)$. Furthermore, the energy levels, E_j, of h can also be degenerated; we denote this degeneration by the number w_j. We then have

Observation 6.1 *To each fixed configuration $(N_1, N_2, \ldots, N_j, \ldots)$ the number of ways of distributing the energies E_j over the N boxes under the above constraints and degeneracies, w_j, is*

$$W = (N!/N_1! \cdots N_j! \cdots) \cdot w_1^{N_1} \cdots w_j^{N_j} \cdots \quad , \quad N = \sum N_j \ , \ E = \sum N_j E_j \tag{90}$$

From the combinatorics of such expressions one knows that there exists a pronounced maximum of W for a special configuration $(N_1, N_2, \ldots, N_j, \ldots)_{max}$ (cf. the above cited literature for more details). The constraints can be implemented via Lagrange multipliers with, in the end, the multiplier β, belonging to the E-constraint, turning out to be something like an *inverse temperature*. It is however important (while usually not openly mentioned in the literature) that for this and other results to hold, $(E - E_0)$ has to

be *macroscopic*, i.e. of order $O(|V|)$. This implies that, with the individual levels, E_j of h, microscopic, most of the occurring N_j are sufficiently large so that *Stirlings formula* can be applied. After some calculations one winds up with the formula

Conclusion 6.2 *Under the assumptions being made we have for the most probable configuration*

$$N_j/N = e^{-\beta E_j} / \sum e^{-\beta E_j} \ , \ \ln W_{max} = N \cdot \ln(\sum_j e^{-\beta E_j} + \beta \cdot E) \qquad (91)$$

(with β only implicitly given by the first equation). In any case, $\ln W_{max}$ turns out to be in general proportional to the volume $|V|$ ($N \sim |V|$) for highly excited states.

These findings have the following consequences for our entanglement problem. With

$$\Psi_E = \sum c_{ij} \, \phi_i^{(E_1)} \otimes \psi_j^{(E_2)} \quad , \quad E_1 + E_2 = E \qquad (92)$$

and $\phi_i^{(E_1)}$, $\psi_j^{(E_2)}$ eigenvectors to the fixed energies E_1 , E_2 of H_1' , H_2', respectively, this is an eigenvector for H' with energy E. Note that, in addition, we could also sum over all possible combinations of E_1 , E_2 with $E_1 + E_2 = E$ but this is not necessary for our argument. We can now make various choices. For one, we can select a very special and simple eigenvector of product type (i.e. all $c_{ij} = 0$ except one), for example:

$$\Psi_E = \phi^{(E_1)} \otimes \psi^{(E_2)} \quad , \quad E_1 + E_2 = E \qquad (93)$$

Its entanglement-entropy is of course zero.

On the other hand, due to the huge degeneracy of all macroscopic levels of H', we can exploit our above conclusion and what we said in the preceding sections about our coarse approximation of entanglement-entropy. It is easy to choose the c_{ij} in such a way that a typical eigenvector to energy E has an entanglement-entropy which is proportional to the volume $|V|$. That is

Conclusion 6.3 *Due to the huge degeneracy of macroscopically excited energy levels of H', the typical eigenvector, belonging to the class of eigenvectors of such an energy level, has an entanglement-entropy of order $O(|V|)$, more specifically*

$$S(W_1) = \alpha_1 \cdot |V_1| = \alpha_2 \cdot |V_2| = S(W_2) \qquad (94)$$

Furthermore, our preceding discussion shows that these states, W_1 , W_2 display features we know from statistical mechanics.

Remarks: i) By "typical" we mean, by randomly selecting one of the admissible eigenvectors from the huge class, we will get such a state with high probability.
ii) We remind the reader of our construction of a vector state belonging to a canonical equilibrium state of system (1) with the help of tensoring with a system (2). Our above findings on higly excited states represent, so to speak, the dual version of this observation. Highly excited states on V have, as we have seen, a tendency to resemble states on, say, V_1 which display a marked statistical mechanical behavior (they are of course not always true equilibrium states).

One could now go on and study systems with a full Hamiltonian, H, starting from such an approximate Hamiltonian H'. As everything is already present in the simpler case, it is clear that nothing strikingly new will happen in the more general situation. On the other hand, the necessary mathematics (perturbation theory) becomes very complex (as we already indicated in the corresponding section), we even had to develop some presumably new approximation schemes. What is called for can already be inferred from the necessary calculations found in some books on ordinary few-body quantum mechanics concerning degenerate levels and/or dense lying energy levels (see for example [20]). We have performed a lot of calculations in this direction but we refrain from representing them in this paper as they are quite tedious and yield, as far as we can see, nothing really new.

7 Low-Lying Excited States

We now discuss the special case that the excited states lie in the vicinity of the groundstate, i.e. instead of energy levels fulfilling

$$\triangle := (E - E_0) = O(|V|) \tag{95}$$

we deal with excitation energies which are much smaller. The same general formula

$$W = (N!/N_1! \cdots N_j! \cdots) \cdot w_1^{N_1} \cdots w_j^{N_j} \cdots \tag{96}$$

holds of course also in this regime but for example Stirlings approximation is no longer applicable as the N_j are in general small. Even if we would ignore this fact (which would presumably only affect the quantitative aspects of some estimates) there exists yet another problem. The energy constraint (we now denote the energy levels of H' by E'_i)

$$\sum E_j \cdot N_j = E'_0 + \triangle = N \cdot E_0 + \triangle \tag{97}$$

with $\triangle \ll |V|$, is more difficult to implement in this regime. It is interesting of analysing the consequences of $\triangle \ll |V|$.

At first glance it seems that we will get the same results as in the previous section by applying the same methods (and in the statistical mechanics literature known to us we have found almost no remark as to possible problems). The method we mentioned and applied previously is indeed very general but there exists a subtle point. The Lagrange multiplier β is only implicitly defined via the constraint

$$E'/N = \sum E_j \cdot e^{-\beta E_j} / \sum e^{-\beta E_j} \tag{98}$$

i.e., it regulates the average energy per box Hamiltonian, h_i, in form of a canonical distribution over the energy levels of h. The E_j are in general not known in detail but one may infer that with $(E' - E'_0) = O(|V|)$ both sides are of the same order for *finite* β so that it is reasonable that we can find some definite value for which the implicit equation can be fulfilled. But we now have $(E' - E'_0)/N \ll 1$ and we conjecture that in this regime the above implicit equation can only be fulfilled for $\beta \gg 1$ or $\beta \to \infty$ (which seems to be quite natural, given the obvious similarities to statistical mechanics. A "thermal" state near the groundstate has by definition a low temperature).

Observation 7.1 *For $(E' - E'_0)$ small, i.e. $(E' - E'_0) \ll O(|V|)$, the parameter β become very large. For these values it becomes difficult to reliably estimate the terms in the occurring variational equations which are now combinations of very large and very small terms. Note in particular that for β large*

$$N_j = N \cdot e^{-\beta E_j} / \sum e^{-\beta E_j} \tag{99}$$

becomes very small compared to N.

Therefore we choose another strategy which is better adapted to this situation. We catalogue the low-lying excitations of H' directly, beginning with the groundstate. We have

Observation 7.2 *1) For the groundstate we have:*

$$E'_0 = N \cdot E_0 \ , \ \textit{no degeneration} \tag{100}$$

2) For one box hamiltonian excited we have:

$$E'_i = (N-1)E_0 + E_i \ , \ W(E'_i) = N \cdot w_i \tag{101}$$

3) Two levels excited; there are two possibilities, $E_i = E_j$ or $E_i \neq E_j$. We have

$$E'_{ii} = (N-2)E_0 + 2E_i \ , \ W(E'_{ii}) = (N \cdot (N-1)/2) \cdot w_i^2 \tag{102}$$

or

$$E'_{ij} = E_i + E_j + (N-2)E_0 \ , \ W(E'_{ij}) = N(N-1) \cdot w_i \cdot w_j \tag{103}$$

etc.

Remark: Note that these results of course coincide with the general formula, inserting the corresponding N_i.

We see the following. Already for the lowest excited levels of H' we have a degeneracy, $W(E'_i) = O(|V|)$. Repeating our previous arguments we infer

Conclusion 7.3 *Already the lowest excited levels of H' have a degeneracy of order $O(|V|)$, entailing that we can construct corresponding eigenstates having an entanglement-entropy of order $O(\ln |V|)$.*

The situation changes slightly if we go over to higher excited levels. For, say, k levels excited the two extreme cases are: 1) all k levels identical or, 2) all levels being different. The intermediate class comprises cases where some of the E_j coincide. We have the following estimate

Observation 7.4 *If k levels are excited, $E_{i_1}, \ldots, E_{i_k}$, with repetitions allowed, we have the estimate*

$$(N!/k! \cdot (N-k)!) w_{i_1} \cdots w_{i_k} \leq W_k \leq (N \cdot (N-1) \cdots (N-k+1)) w_{i_1} \cdots w_{i_k} \tag{104}$$

As, by assumption, the local h_i have only finite spectrum, the possible degeneracies are also finite and can be bounded by some constant. This yields:

Corollary 7.5 *We have*

$$(N!/k! \cdot (N-k)!) \leq W_k \leq C^k \cdot (N \cdot (N-1) \cdots (N-k+1)) \tag{105}$$

For N very large compared to k, this entails

$$W_k = O(N^k) \quad \textit{and} \quad \ln W_k = O(k \cdot \ln N) = O(k \cdot \ln |V|) \tag{106}$$

Remark: What we have said at the end of the preceding sections applies also here. When we go over from our Hamiltonian H' to the full, translation invariant Hamiltonian H, we have to perform a tedious perturbation analysis in order to compare the results. We again refrain from doing this as it does not change our general results.

References

[1] T.Jacobson,D.Marolf,C.Rovelli: "Black Hole Entropy: Inside or Out?", Int.J.Theor.Phys. 44(2005)1807, hep-th/0501103

[2] R.D.Sorkin: "Ten Theses on Black Hole Entropy", Stud.Hist.Philos.Mod.Phys. 36(2005)291, hep-th/0504037

[3] R.Bousso: "The Holographic Principle", Rev.Mod.Phys. 74(2002)825, hep-th/0203101

[4] M.Requardt: "Planck Fluctuations, Measurement Uncertainties, and the Holographic Principle, gr-qc/0505019

[5] L.Bombelli,K.Kaul,J.Lee,R.Sorkin: "Quantum Source of Entropy for Black Holes", Phys.Rev. D34(1986)373

[6] M.Srednicki: "Entropy and Area", Phys.Rev.Lett. 71(1993)666, hep-th/9303048

[7] B.Schroer: "More on Area Density of Localisation-Entropy and Problematization of Black Hole Entropy", hep-th/0511291

[8] P.Calabrese,J.Cardy: "Entanglement Entropy and Quantum Field Theory: A Non-Technical Introduction", Conference "Entanglement in Physical and Information Sciences", Pisa Dec. 2004, quant-ph/0505193

[9] P.Calabrese,J.Cardy: "Entanglement Entropy and Quantum Field Theory", J.Stat.Mech. P06002 (2004), hep-th/0405152

[10] I.Peschel: "On the Entanglement Entropy for a XY Spin Chain", J.Stat.Mech. P12005 (2004), cond-mat/0410416

[11] M.Reed,B.Simon: "Methods of Modern Mathematical Physics" vol. I, Academ.Pr., London 1980

[12] W.Thirring: "Lehrbuch der Mathematischen Physik", vol.4, "Quantenmechanik grosser Systeme", Springer, Wien 1980

[13] E.Schmidt: Math.Annalen 63(1907)433

[14] J.von Neumann: "Mathematische Grundlagen der Quantenmechanik", Springer, Berlin 1932

[15] A.Ekert,P.L.Knight: Am.J.Phys. 63(1995)415

[16] L.D.Landau,E.M.Lifschitz: "Statistische Physik", Akademie-Verlag, Berlin 1966

[17] H.Baumgaertel: "Endlich-dimensionale Analytische Stoerungstheorie", Akadem. Verlagsgesellschaft, Berlin 1972

[18] N.I.Achieser,I.M.Glasmann: "Theorie der Linearen Operatoren im Hilbert-Raum", Akademie-Verlag, Berlin 1968

[19] T.Kato: "Perturbation Theory for Linear Operators", Springer, N.Y. 1966

[20] A.Dawydow: "Quantenmechanik" sections 49, 50, Deutscher Verlag der Wissenschaften, Berlin 1974

[21] F.Riesz,B.SZ.-Nagy: "Vorlesungen ueber Funktionalanalysis", Deutscher Verlag der Wissenschaften, Berlin 1956

[22] A.Weinstein,W.Stenger: "Intermediate Problems for Eigenvalues", Academic Pr., N.Y.1972

[23] R.Becker: "Theorie der Waerme", Springer, Berlin 1966

[24] R.C.Tolman: "The Principles of Statistical mechanics", Dover, N.Y. 1979

[25] E.Schroedinger: "Statistical Thermodynamics", Cambridge Univ. Pr., Cambridge 1946

[26] R.H.Fowler: "Statistical Mechanics", Cambridge Univ. Pr., Cambridge 1936